Supplementary Data for:

Ruthenium Complex with a 6-Memebered *N*-Heterocyclic Carbene Ligand

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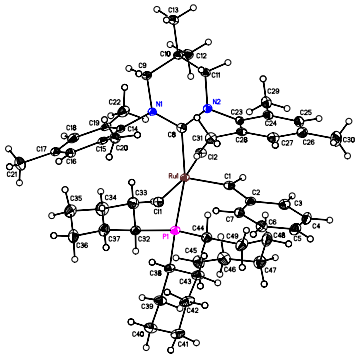
Contents



JSY01

Note: The crystallographic data has been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 186478. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 186478."

Table 1. Crystal data and structure refinement for JSY01 (CCDC 186478).

Empirical formula	$C_{49}H_{71}Cl_2N_2PRu$
Formula weight	891.02
Crystallization Solvent	Pentane/dichloromethane
Crystal Habit	Plate
Crystal size	0.26 x 0.22 x 0.07 mm^3
Crystal color	Dichroic - Yellow/brown to orange

Data Collection

Preliminary Photos	Rotation
Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	98(2) K
θ range for 38647 reflections used in lattice determination	2.29 to 28.26°
Unit cell dimensions	a = 18.3317(7) Å b = 12.5852(5) Å β= 104.3240(10)° c = 19.9966(7) Å
Volume	4470.0(3) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/n$
Density (calculated)	1.324 Mg/m^3
F(000)	1888
Data collection program	Bruker SMART v5.054
θ range for data collection	1.74 to 28.48°
Completeness to θ = 28.48°	94.5 %
Index ranges	$-24 \le h \le 24$, $-16 \le k \le 16$, $-26 \le l \le 26$
Data collection scan type	ω scans at 7 ϕ settings
Data reduction program	Bruker SAINT v6.022
Reflections collected	90760
Independent reflections	10676 [R_{int}= 0.0580]
Absorption coefficient	0.542 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9631 and 0.8720

Table 1 (cont.)

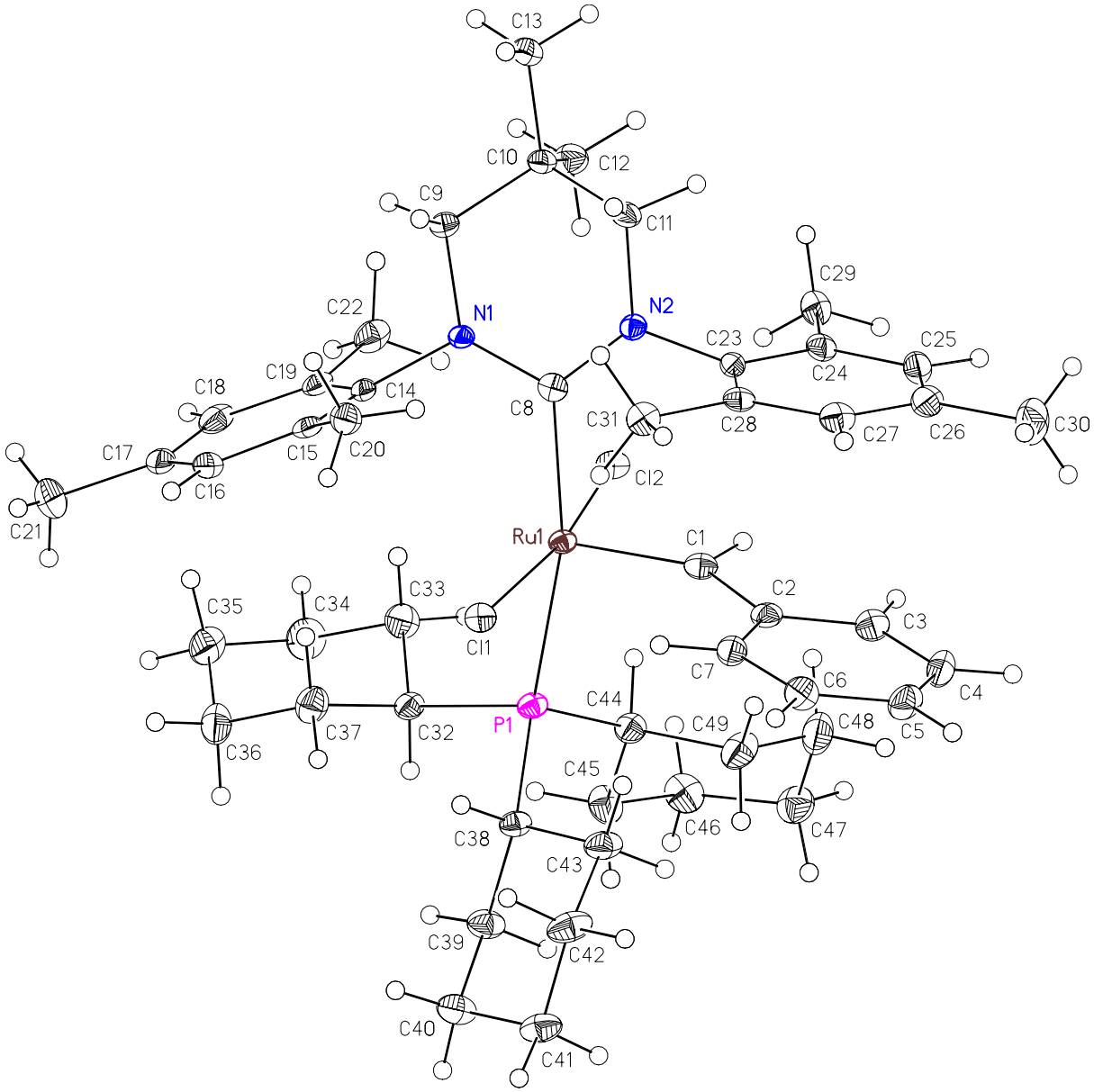
Structure solution and Refinement

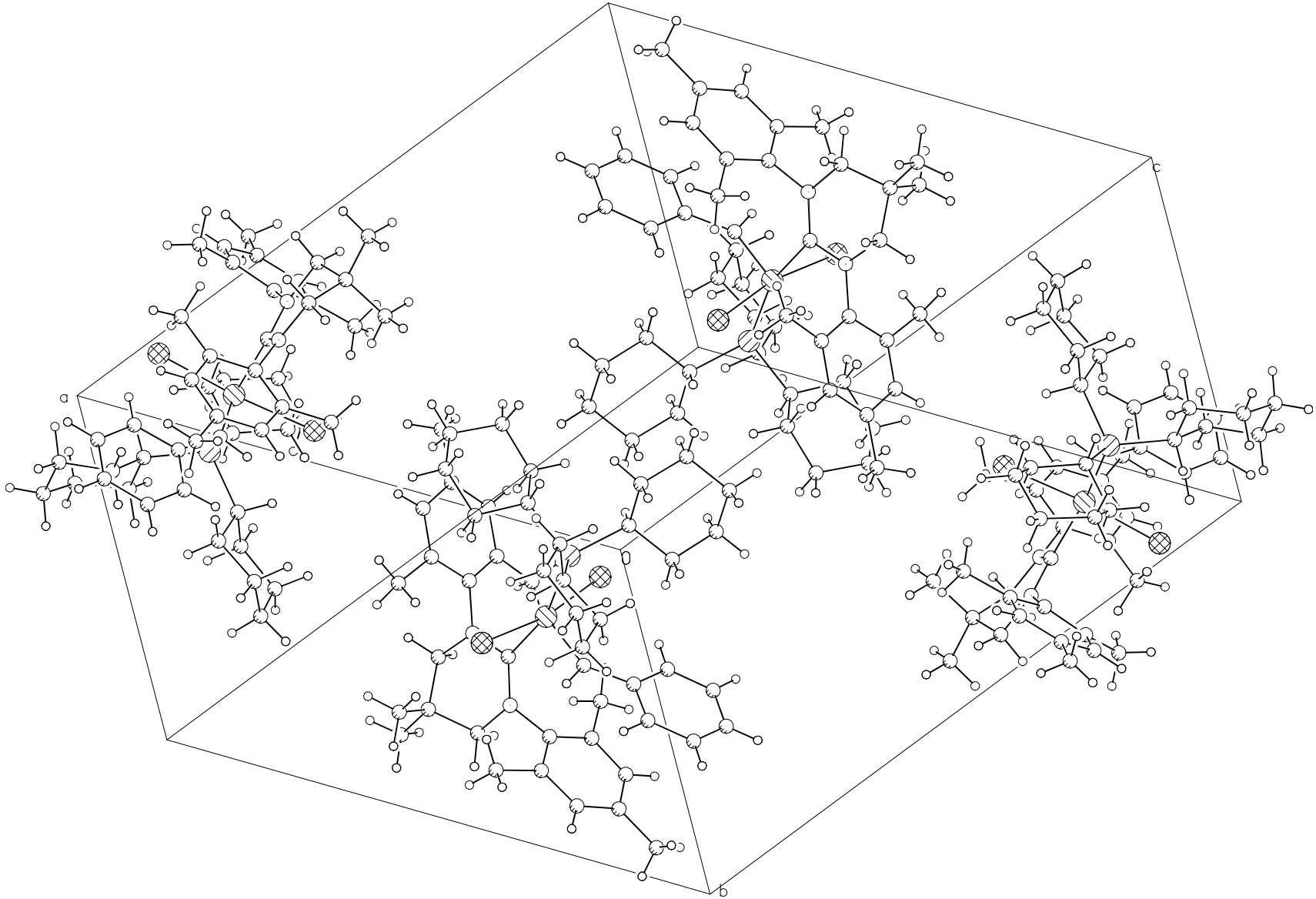
Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	10676 / 0 / 780
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.765
Final R indices [$I>2\sigma(I)$, 8468 reflections]	R1 = 0.0305, *w*R2 = 0.0521
R indices (all data)	R1 = 0.0453, *w*R2 = 0.0537
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	0.828 and -0.637 e.Å^{-3}

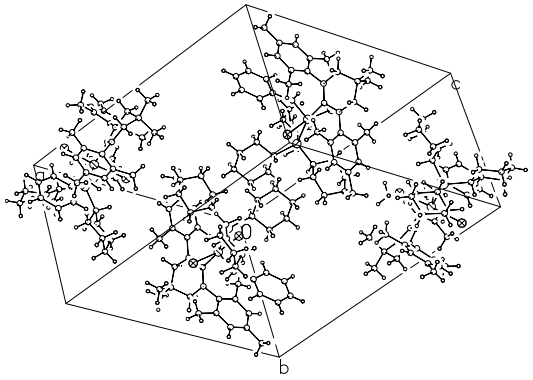
Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


C13
C10
C12
C9
C11
C29
C22
N1
N2
C23
C25
C24
C19
C18
C14
C8
C31
C28
C27
C26
C30
C17
C15
C20
C12
C16
C21
Ru1
C1
C35
C34
C33
C2
C3
C11
C7
C6
C4
C44
C49
C48
C5
P1
C37
C32
C36
C45
C46
C47
C38
C43
C39
C42
C40
C41




c
b

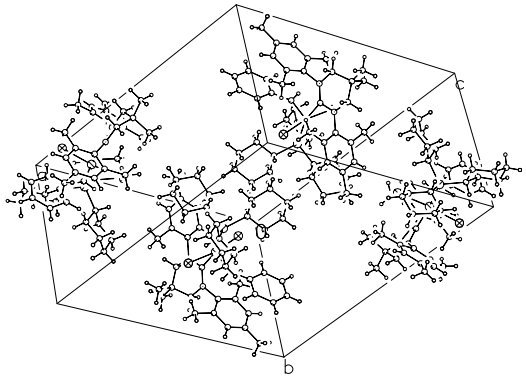

c
b

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for JSY01 (CCDC 186478). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	9720(1)	2436(1)	2256(1)	11(1)
Cl(1)	10597(1)	1258(1)	1934(1)	16(1)
Cl(2)	8678(1)	3334(1)	2551(1)	15(1)
P(1)	8984(1)	2374(1)	1055(1)	13(1)
N(1)	9873(1)	1315(1)	3603(1)	11(1)
N(2)	10479(1)	2918(1)	3792(1)	12(1)
C(1)	10123(1)	3753(1)	2184(1)	14(1)
C(2)	10788(1)	4212(1)	2000(1)	15(1)
C(3)	10811(1)	5321(2)	1945(1)	18(1)
C(4)	11413(1)	5831(2)	1786(1)	20(1)
C(5)	12015(1)	5243(2)	1685(1)	22(1)
C(6)	12003(1)	4151(2)	1734(1)	19(1)
C(7)	11397(1)	3630(2)	1888(1)	16(1)
C(8)	10110(1)	2197(1)	3327(1)	12(1)
C(9)	10006(1)	1093(1)	4350(1)	14(1)
C(10)	10069(1)	2101(1)	4774(1)	15(1)
C(11)	10643(1)	2782(1)	4549(1)	15(1)
C(12)	9312(1)	2672(2)	4644(1)	19(1)
C(13)	10358(1)	1842(2)	5538(1)	21(1)
C(14)	9564(1)	391(1)	3196(1)	13(1)
C(15)	10054(1)	-373(1)	3049(1)	15(1)
C(16)	9748(1)	-1318(2)	2739(1)	19(1)
C(17)	8989(1)	-1549(1)	2615(1)	21(1)
C(18)	8522(1)	-796(2)	2800(1)	20(1)
C(19)	8789(1)	180(1)	3082(1)	15(1)
C(20)	10897(1)	-266(2)	3270(1)	18(1)
C(21)	8674(2)	-2596(2)	2308(1)	33(1)
C(22)	8258(1)	943(2)	3289(1)	20(1)
C(23)	10906(1)	3817(1)	3637(1)	13(1)
C(24)	10647(1)	4844(1)	3702(1)	15(1)
C(25)	11131(1)	5688(2)	3670(1)	19(1)
C(26)	11857(1)	5534(2)	3596(1)	20(1)
C(27)	12090(1)	4503(2)	3531(1)	17(1)
C(28)	11630(1)	3630(1)	3555(1)	14(1)
C(29)	9879(1)	5058(2)	3805(1)	19(1)
C(30)	12370(1)	6461(2)	3570(1)	30(1)
C(31)	11902(1)	2523(2)	3478(1)	17(1)
C(32)	8243(1)	1335(1)	903(1)	15(1)
C(33)	7673(1)	1461(2)	1339(1)	21(1)
C(34)	7023(1)	677(2)	1092(1)	25(1)
C(35)	7293(1)	-463(2)	1097(1)	24(1)
C(36)	7904(1)	-584(2)	712(1)	25(1)
C(37)	8550(1)	199(2)	966(1)	21(1)
C(38)	9489(1)	2014(2)	391(1)	15(1)
C(39)	9011(1)	1871(2)	-350(1)	20(1)
C(40)	9480(1)	1392(2)	-809(1)	24(1)
C(41)	10188(1)	2033(2)	-787(1)	22(1)

C(42)	10647(1)	2176(2)	-45(1)	24(1)
C(43)	10173(1)	2700(2)	390(1)	21(1)
C(44)	8429(1)	3605(1)	807(1)	16(1)
C(45)	7755(1)	3578(2)	181(1)	22(1)
C(46)	7277(1)	4579(2)	165(1)	23(1)
C(47)	7725(1)	5595(2)	183(1)	24(1)
C(48)	8424(1)	5583(2)	779(1)	28(1)
C(49)	8897(1)	4592(2)	759(1)	23(1)

Table 3. Selected bond lengths [Å] and angles [°] for JSY01 (CCDC 186478).

Ru(1)-C(1)	1.8353(18)	C(1)-Ru(1)-C(8)	99.62(7)
Ru(1)-C(8)	2.1059(17)	C(1)-Ru(1)-Cl(1)	103.19(6)
Ru(1)-Cl(1)	2.3899(5)	C(8)-Ru(1)-Cl(1)	95.92(4)
Ru(1)-Cl(2)	2.4151(4)	C(1)-Ru(1)-Cl(2)	87.42(6)
Ru(1)-P(1)	2.4470(4)	C(8)-Ru(1)-Cl(2)	84.75(4)
		Cl(1)-Ru(1)-Cl(2)	169.063(16)
		C(1)-Ru(1)-P(1)	94.96(5)
		C(8)-Ru(1)-P(1)	163.71(5)
		Cl(1)-Ru(1)-P(1)	87.750(15)
		Cl(2)-Ru(1)-P(1)	88.696(15)

Table 4. Bond lengths [Å] and angles [°] for JSY01 (CCDC 186478).

Ru(1)-C(1)	1.8353(18)	C(19)-C(22)	1.496(3)
Ru(1)-C(8)	2.1059(17)	C(20)-H(20A)	0.958(19)
Ru(1)-Cl(1)	2.3899(5)	C(20)-H(20B)	0.907(18)
Ru(1)-Cl(2)	2.4151(4)	C(20)-H(20C)	0.932(19)
Ru(1)-P(1)	2.4470(4)	C(21)-H(21A)	0.94(3)
P(1)-C(44)	1.8521(18)	C(21)-H(21B)	0.86(3)
P(1)-C(32)	1.8547(18)	C(21)-H(21C)	0.92(3)
P(1)-C(38)	1.8544(18)	C(22)-H(22A)	0.941(19)
N(1)-C(8)	1.357(2)	C(22)-H(22B)	0.94(2)
N(1)-C(14)	1.452(2)	C(22)-H(22C)	0.977(19)
N(1)-C(9)	1.479(2)	C(23)-C(24)	1.394(2)
N(2)-C(8)	1.354(2)	C(23)-C(28)	1.397(2)
N(2)-C(23)	1.452(2)	C(24)-C(25)	1.395(2)
N(2)-C(11)	1.479(2)	C(24)-C(29)	1.498(2)
C(1)-C(2)	1.475(2)	C(25)-C(26)	1.389(3)
C(1)-H(1)	0.946(17)	C(25)-H(25)	0.972(18)
C(2)-C(7)	1.400(2)	C(26)-C(27)	1.382(3)
C(2)-C(3)	1.401(2)	C(26)-C(30)	1.507(3)
C(3)-C(4)	1.381(3)	C(27)-C(28)	1.393(2)
C(3)-H(3)	0.976(17)	C(27)-H(27)	0.947(18)
C(4)-C(5)	1.384(3)	C(28)-C(31)	1.500(2)
C(4)-H(4)	0.955(16)	C(29)-H(29A)	0.96(2)
C(5)-C(6)	1.378(3)	C(29)-H(29B)	0.91(2)
C(5)-H(5)	0.951(18)	C(29)-H(29C)	0.985(19)
C(6)-C(7)	1.387(2)	C(30)-H(30A)	0.91(3)
C(6)-H(6)	0.956(18)	C(30)-H(30B)	0.96(3)
C(7)-H(7)	0.964(16)	C(30)-H(30C)	0.88(3)
C(9)-C(10)	1.514(2)	C(31)-H(31A)	0.93(2)
C(9)-H(9A)	0.971(17)	C(31)-H(31B)	0.993(18)
C(9)-H(9B)	0.982(16)	C(31)-H(31C)	0.989(19)
C(10)-C(11)	1.510(2)	C(32)-C(33)	1.527(3)
C(10)-C(13)	1.523(2)	C(32)-C(37)	1.531(3)
C(10)-C(12)	1.525(3)	C(32)-H(32)	0.936(16)
C(11)-H(11A)	1.014(16)	C(33)-C(34)	1.531(3)
C(11)-H(11B)	0.945(17)	C(33)-H(33A)	0.92(2)
C(12)-H(12A)	0.991(19)	C(33)-H(33B)	0.987(19)
C(12)-H(12B)	0.970(19)	C(34)-C(35)	1.516(3)
C(12)-H(12C)	0.95(2)	C(34)-H(34A)	0.979(19)
C(13)-H(13A)	1.004(18)	C(34)-H(34B)	0.95(2)
C(13)-H(13B)	0.947(19)	C(35)-C(36)	1.517(3)
C(13)-H(13C)	0.94(2)	C(35)-H(35A)	0.95(2)
C(14)-C(15)	1.397(2)	C(35)-H(35B)	0.969(19)
C(14)-C(19)	1.407(2)	C(36)-C(37)	1.527(3)
C(15)-C(16)	1.392(2)	C(36)-H(36A)	1.00(2)
C(15)-C(20)	1.505(3)	C(36)-H(36B)	0.928(18)
C(16)-C(17)	1.384(3)	C(37)-H(37A)	0.987(19)
C(16)-H(16)	0.924(17)	C(37)-H(37B)	0.974(19)
C(17)-C(18)	1.386(3)	C(38)-C(43)	1.522(3)
C(17)-C(21)	1.508(3)	C(38)-C(39)	1.534(2)
C(18)-C(19)	1.388(2)	C(38)-H(38)	0.917(16)
C(18)-H(18)	0.894(17)	C(39)-C(40)	1.529(3)

C(39)-H(39A)	0.988(18)	C(2)-C(1)-H(1)	109.7(11)
C(39)-H(39B)	0.966(19)	Ru(1)-C(1)-H(1)	111.9(11)
C(40)-C(41)	1.519(3)	C(7)-C(2)-C(3)	117.84(17)
C(40)-H(40A)	0.933(18)	C(7)-C(2)-C(1)	125.20(16)
C(40)-H(40B)	0.924(19)	C(3)-C(2)-C(1)	116.95(16)
C(41)-C(42)	1.525(3)	C(4)-C(3)-C(2)	121.57(18)
C(41)-H(41A)	0.926(18)	C(4)-C(3)-H(3)	121.3(10)
C(41)-H(41B)	0.956(18)	C(2)-C(3)-H(3)	117.1(10)
C(42)-C(43)	1.524(3)	C(3)-C(4)-C(5)	119.72(18)
C(42)-H(42A)	1.01(2)	C(3)-C(4)-H(4)	119.5(10)
C(42)-H(42B)	1.000(19)	C(5)-C(4)-H(4)	120.8(10)
C(43)-H(43A)	0.930(18)	C(6)-C(5)-C(4)	119.69(18)
C(43)-H(43B)	0.978(17)	C(6)-C(5)-H(5)	120.5(11)
C(44)-C(45)	1.525(2)	C(4)-C(5)-H(5)	119.8(11)
C(44)-C(49)	1.526(3)	C(5)-C(6)-C(7)	121.02(18)
C(44)-H(44)	1.003(17)	C(5)-C(6)-H(6)	120.6(11)
C(45)-C(46)	1.530(3)	C(7)-C(6)-H(6)	118.3(11)
C(45)-H(45A)	0.988(19)	C(6)-C(7)-C(2)	120.15(17)
C(45)-H(45B)	1.02(2)	C(6)-C(7)-H(7)	119.6(10)
C(46)-C(47)	1.516(3)	C(2)-C(7)-H(7)	120.3(10)
C(46)-H(46A)	0.92(2)	N(2)-C(8)-N(1)	115.15(15)
C(46)-H(46B)	0.98(2)	N(2)-C(8)-Ru(1)	126.04(12)
C(47)-C(48)	1.518(3)	N(1)-C(8)-Ru(1)	117.90(12)
C(47)-H(47A)	0.997(18)	N(1)-C(9)-C(10)	112.13(14)
C(47)-H(47B)	0.924(18)	N(1)-C(9)-H(9A)	106.4(10)
C(48)-C(49)	1.525(3)	C(10)-C(9)-H(9A)	111.8(10)
C(48)-H(48A)	0.96(2)	N(1)-C(9)-H(9B)	107.0(9)
C(48)-H(48B)	1.03(2)	C(10)-C(9)-H(9B)	110.8(9)
C(49)-H(49A)	0.93(2)	H(9A)-C(9)-H(9B)	108.4(14)
C(49)-H(49B)	0.951(19)	C(11)-C(10)-C(9)	105.74(15)
		C(11)-C(10)-C(13)	108.90(15)
C(1)-Ru(1)-C(8)	99.62(7)	C(9)-C(10)-C(13)	109.93(15)
C(1)-Ru(1)-Cl(1)	103.19(6)	C(11)-C(10)-C(12)	110.71(15)
C(8)-Ru(1)-Cl(1)	95.92(4)	C(9)-C(10)-C(12)	111.07(15)
C(1)-Ru(1)-Cl(2)	87.42(6)	C(13)-C(10)-C(12)	110.38(16)
C(8)-Ru(1)-Cl(2)	84.75(4)	N(2)-C(11)-C(10)	112.92(14)
Cl(1)-Ru(1)-Cl(2)	169.063(16)	N(2)-C(11)-H(11A)	106.4(9)
C(1)-Ru(1)-P(1)	94.96(5)	C(10)-C(11)-H(11A)	111.0(9)
C(8)-Ru(1)-P(1)	163.71(5)	N(2)-C(11)-H(11B)	106.9(10)
Cl(1)-Ru(1)-P(1)	87.750(15)	C(10)-C(11)-H(11B)	111.3(10)
Cl(2)-Ru(1)-P(1)	88.696(15)	H(11A)-C(11)-H(11B)	108.0(14)
C(44)-P(1)-C(32)	102.41(8)	C(10)-C(12)-H(12A)	111.9(11)
C(44)-P(1)-C(38)	110.50(9)	C(10)-C(12)-H(12B)	112.1(11)
C(32)-P(1)-C(38)	100.65(8)	H(12A)-C(12)-H(12B)	108.0(15)
C(44)-P(1)-Ru(1)	111.71(6)	C(10)-C(12)-H(12C)	111.6(12)
C(32)-P(1)-Ru(1)	112.77(6)	H(12A)-C(12)-H(12C)	106.9(16)
C(38)-P(1)-Ru(1)	117.32(6)	H(12B)-C(12)-H(12C)	106.0(16)
C(8)-N(1)-C(14)	123.15(14)	C(10)-C(13)-H(13A)	111.7(10)
C(8)-N(1)-C(9)	125.14(14)	C(10)-C(13)-H(13B)	108.1(11)
C(14)-N(1)-C(9)	110.99(13)	H(13A)-C(13)-H(13B)	110.4(15)
C(8)-N(2)-C(23)	125.45(14)	C(10)-C(13)-H(13C)	109.8(12)
C(8)-N(2)-C(11)	124.44(14)	H(13A)-C(13)-H(13C)	109.3(16)
C(23)-N(2)-C(11)	108.95(13)	H(13B)-C(13)-H(13C)	107.5(16)
C(2)-C(1)-Ru(1)	138.36(14)	C(15)-C(14)-C(19)	120.81(16)

C(15)-C(14)-N(1)	119.17(15)	C(24)-C(29)-H(29B)	112.2(13)
C(19)-C(14)-N(1)	118.74(15)	H(29A)-C(29)-H(29B)	107.4(17)
C(16)-C(15)-C(14)	118.22(17)	C(24)-C(29)-H(29C)	109.5(11)
C(16)-C(15)-C(20)	118.58(17)	H(29A)-C(29)-H(29C)	110.2(15)
C(14)-C(15)-C(20)	122.95(16)	H(29B)-C(29)-H(29C)	106.2(16)
C(17)-C(16)-C(15)	122.34(18)	C(26)-C(30)-H(30A)	114.3(16)
C(17)-C(16)-H(16)	119.3(11)	C(26)-C(30)-H(30B)	109.3(15)
C(15)-C(16)-H(16)	118.3(11)	H(30A)-C(30)-H(30B)	111(2)
C(16)-C(17)-C(18)	117.95(17)	C(26)-C(30)-H(30C)	109.4(17)
C(16)-C(17)-C(21)	121.52(19)	H(30A)-C(30)-H(30C)	104(2)
C(18)-C(17)-C(21)	120.51(19)	H(30B)-C(30)-H(30C)	108(2)
C(17)-C(18)-C(19)	122.32(18)	C(28)-C(31)-H(31A)	109.0(12)
C(17)-C(18)-H(18)	120.7(11)	C(28)-C(31)-H(31B)	112.6(10)
C(19)-C(18)-H(18)	116.9(11)	H(31A)-C(31)-H(31B)	109.0(16)
C(18)-C(19)-C(14)	118.18(17)	C(28)-C(31)-H(31C)	110.7(11)
C(18)-C(19)-C(22)	119.50(17)	H(31A)-C(31)-H(31C)	107.7(16)
C(14)-C(19)-C(22)	122.23(16)	H(31B)-C(31)-H(31C)	107.7(15)
C(15)-C(20)-H(20A)	110.6(11)	C(33)-C(32)-C(37)	109.83(15)
C(15)-C(20)-H(20B)	112.7(11)	C(33)-C(32)-P(1)	114.17(13)
H(20A)-C(20)-H(20B)	107.8(16)	C(37)-C(32)-P(1)	113.96(13)
C(15)-C(20)-H(20C)	110.3(11)	C(33)-C(32)-H(32)	108.2(10)
H(20A)-C(20)-H(20C)	105.9(15)	C(37)-C(32)-H(32)	106.4(10)
H(20B)-C(20)-H(20C)	109.4(16)	P(1)-C(32)-H(32)	103.6(10)
C(17)-C(21)-H(21A)	110.0(16)	C(32)-C(33)-C(34)	109.69(16)
C(17)-C(21)-H(21B)	112.8(18)	C(32)-C(33)-H(33A)	110.4(12)
H(21A)-C(21)-H(21B)	111(2)	C(34)-C(33)-H(33A)	109.4(12)
C(17)-C(21)-H(21C)	111.8(16)	C(32)-C(33)-H(33B)	112.5(11)
H(21A)-C(21)-H(21C)	101(2)	C(34)-C(33)-H(33B)	111.0(11)
H(21B)-C(21)-H(21C)	110(2)	H(33A)-C(33)-H(33B)	103.6(15)
C(19)-C(22)-H(22A)	108.4(11)	C(35)-C(34)-C(33)	112.46(17)
C(19)-C(22)-H(22B)	113.3(12)	C(35)-C(34)-H(34A)	108.9(11)
H(22A)-C(22)-H(22B)	110.0(16)	C(33)-C(34)-H(34A)	107.1(11)
C(19)-C(22)-H(22C)	108.7(11)	C(35)-C(34)-H(34B)	110.5(12)
H(22A)-C(22)-H(22C)	108.7(15)	C(33)-C(34)-H(34B)	109.2(12)
H(22B)-C(22)-H(22C)	107.7(15)	H(34A)-C(34)-H(34B)	108.5(16)
C(24)-C(23)-C(28)	121.44(16)	C(34)-C(35)-C(36)	111.88(17)
C(24)-C(23)-N(2)	119.30(15)	C(34)-C(35)-H(35A)	109.8(12)
C(28)-C(23)-N(2)	118.14(15)	C(36)-C(35)-H(35A)	109.7(12)
C(23)-C(24)-C(25)	117.86(17)	C(34)-C(35)-H(35B)	109.5(11)
C(23)-C(24)-C(29)	122.15(16)	C(36)-C(35)-H(35B)	112.5(11)
C(25)-C(24)-C(29)	119.99(16)	H(35A)-C(35)-H(35B)	103.1(15)
C(26)-C(25)-C(24)	122.35(17)	C(35)-C(36)-C(37)	112.05(17)
C(26)-C(25)-H(25)	119.8(11)	C(35)-C(36)-H(36A)	110.3(11)
C(24)-C(25)-H(25)	117.8(11)	C(37)-C(36)-H(36A)	108.2(11)
C(27)-C(26)-C(25)	117.91(17)	C(35)-C(36)-H(36B)	108.1(11)
C(27)-C(26)-C(30)	120.92(19)	C(37)-C(36)-H(36B)	112.2(11)
C(25)-C(26)-C(30)	121.15(18)	H(36A)-C(36)-H(36B)	105.8(15)
C(26)-C(27)-C(28)	122.22(18)	C(36)-C(37)-C(32)	109.63(16)
C(26)-C(27)-H(27)	118.0(11)	C(36)-C(37)-H(37A)	109.7(11)
C(28)-C(27)-H(27)	119.7(11)	C(32)-C(37)-H(37A)	109.8(11)
C(27)-C(28)-C(23)	118.19(16)	C(36)-C(37)-H(37B)	109.8(11)
C(27)-C(28)-C(31)	120.64(16)	C(32)-C(37)-H(37B)	108.7(11)
C(23)-C(28)-C(31)	121.16(16)	H(37A)-C(37)-H(37B)	109.2(15)
C(24)-C(29)-H(29A)	111.2(12)	C(43)-C(38)-C(39)	109.87(15)

C(43)-C(38)-P(1)	114.81(13)	C(45)-C(44)-P(1)	118.75(13)
C(39)-C(38)-P(1)	116.96(13)	C(49)-C(44)-P(1)	114.69(13)
C(43)-C(38)-H(38)	104.1(10)	C(45)-C(44)-H(44)	105.7(10)
C(39)-C(38)-H(38)	108.4(10)	C(49)-C(44)-H(44)	106.1(10)
P(1)-C(38)-H(38)	101.3(10)	P(1)-C(44)-H(44)	101.4(10)
C(40)-C(39)-C(38)	110.77(16)	C(44)-C(45)-C(46)	110.06(16)
C(40)-C(39)-H(39A)	107.5(11)	C(44)-C(45)-H(45A)	109.6(11)
C(38)-C(39)-H(39A)	108.5(11)	C(46)-C(45)-H(45A)	109.8(11)
C(40)-C(39)-H(39B)	109.1(11)	C(44)-C(45)-H(45B)	110.4(11)
C(38)-C(39)-H(39B)	113.1(11)	C(46)-C(45)-H(45B)	107.2(11)
H(39A)-C(39)-H(39B)	107.6(15)	H(45A)-C(45)-H(45B)	109.8(15)
C(41)-C(40)-C(39)	112.14(17)	C(47)-C(46)-C(45)	112.96(17)
C(41)-C(40)-H(40A)	109.0(11)	C(47)-C(46)-H(46A)	108.9(12)
C(39)-C(40)-H(40A)	109.0(11)	C(45)-C(46)-H(46A)	109.9(13)
C(41)-C(40)-H(40B)	110.1(11)	C(47)-C(46)-H(46B)	110.0(11)
C(39)-C(40)-H(40B)	109.6(11)	C(45)-C(46)-H(46B)	108.1(11)
H(40A)-C(40)-H(40B)	106.9(15)	H(46A)-C(46)-H(46B)	106.8(17)
C(40)-C(41)-C(42)	110.66(17)	C(46)-C(47)-C(48)	110.91(17)
C(40)-C(41)-H(41A)	109.1(12)	C(46)-C(47)-H(47A)	109.6(10)
C(42)-C(41)-H(41A)	110.0(12)	C(48)-C(47)-H(47A)	111.3(10)
C(40)-C(41)-H(41B)	110.8(11)	C(46)-C(47)-H(47B)	110.6(11)
C(42)-C(41)-H(41B)	109.6(11)	C(48)-C(47)-H(47B)	109.0(11)
H(41A)-C(41)-H(41B)	106.6(16)	H(47A)-C(47)-H(47B)	105.3(15)
C(43)-C(42)-C(41)	110.54(16)	C(47)-C(48)-C(49)	111.25(18)
C(43)-C(42)-H(42A)	107.3(11)	C(47)-C(48)-H(48A)	111.0(12)
C(41)-C(42)-H(42A)	110.5(11)	C(49)-C(48)-H(48A)	106.0(12)
C(43)-C(42)-H(42B)	110.9(11)	C(47)-C(48)-H(48B)	107.7(11)
C(41)-C(42)-H(42B)	111.0(10)	C(49)-C(48)-H(48B)	109.5(11)
H(42A)-C(42)-H(42B)	106.5(15)	H(48A)-C(48)-H(48B)	111.4(16)
C(38)-C(43)-C(42)	109.94(16)	C(48)-C(49)-C(44)	109.33(17)
C(38)-C(43)-H(43A)	111.3(11)	C(48)-C(49)-H(49A)	110.1(12)
C(42)-C(43)-H(43A)	108.9(11)	C(44)-C(49)-H(49A)	108.8(12)
C(38)-C(43)-H(43B)	110.1(10)	C(48)-C(49)-H(49B)	109.9(11)
C(42)-C(43)-H(43B)	110.1(10)	C(44)-C(49)-H(49B)	107.3(12)
H(43A)-C(43)-H(43B)	106.4(14)	H(49A)-C(49)-H(49B)	111.3(17)
C(45)-C(44)-C(49)	108.69(16)		

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for JSY01 (CCDC 186478). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	90(1)	141(1)	89(1)	9(1)	10(1)	-7(1)
Cl(1)	154(2)	170(2)	148(2)	3(2)	39(2)	8(2)
Cl(2)	118(2)	205(2)	138(2)	2(2)	32(2)	10(2)
P(1)	102(2)	171(2)	103(2)	12(2)	10(2)	-18(2)
N(1)	120(8)	125(7)	79(7)	4(6)	6(6)	-20(6)
N(2)	115(7)	118(7)	105(8)	13(6)	8(6)	2(6)
C(1)	116(9)	188(10)	106(9)	9(7)	-1(7)	23(8)
C(2)	158(10)	183(10)	93(9)	13(7)	1(7)	-10(8)
C(3)	161(10)	196(10)	165(10)	17(8)	15(8)	17(8)
C(4)	225(11)	147(10)	234(11)	33(8)	50(9)	-22(8)
C(5)	195(11)	251(11)	227(11)	23(8)	79(9)	-77(9)
C(6)	167(10)	215(10)	204(11)	-14(8)	56(8)	-12(8)
C(7)	164(10)	165(10)	144(10)	10(8)	6(8)	-13(8)
C(8)	75(8)	140(9)	139(9)	0(7)	24(7)	41(7)
C(9)	162(10)	148(10)	102(9)	21(7)	12(8)	4(8)
C(10)	197(10)	140(9)	93(9)	1(7)	26(8)	8(7)
C(11)	164(10)	166(10)	97(9)	-8(7)	-6(7)	14(8)
C(12)	202(10)	208(11)	173(10)	-4(9)	69(8)	12(8)
C(13)	325(13)	167(11)	128(10)	-13(8)	38(9)	-1(9)
C(14)	178(10)	123(9)	77(9)	14(7)	8(7)	-35(7)
C(15)	199(10)	167(9)	81(9)	34(7)	31(7)	-19(8)
C(16)	297(12)	153(10)	124(10)	5(8)	61(8)	10(9)
C(17)	314(12)	187(10)	91(9)	14(8)	-2(8)	-92(9)
C(18)	179(11)	270(11)	130(10)	51(8)	-12(8)	-102(9)
C(19)	173(10)	184(10)	87(9)	44(7)	8(7)	-37(8)
C(20)	207(11)	160(10)	173(11)	4(9)	39(9)	25(8)
C(21)	450(15)	239(12)	264(12)	-66(11)	46(11)	-144(12)
C(22)	144(11)	262(12)	191(11)	41(9)	33(9)	-56(9)
C(23)	137(9)	132(9)	91(9)	-5(7)	-6(7)	-45(7)
C(24)	155(10)	163(9)	113(9)	-11(7)	-7(7)	-7(7)
C(25)	251(11)	136(10)	167(10)	-7(8)	15(8)	-6(8)
C(26)	193(10)	222(10)	152(10)	1(8)	-1(8)	-71(8)
C(27)	109(10)	245(11)	149(10)	-3(8)	3(8)	-26(8)
C(28)	125(9)	181(9)	82(9)	4(7)	-18(7)	4(7)
C(29)	189(11)	159(10)	209(11)	-18(9)	36(9)	6(8)
C(30)	286(14)	242(12)	372(15)	-5(11)	60(11)	-108(10)
C(31)	124(9)	197(10)	187(10)	8(9)	21(8)	15(9)
C(32)	133(10)	172(10)	119(10)	17(7)	4(8)	-29(7)
C(33)	172(10)	239(11)	211(11)	-20(9)	57(9)	-51(8)
C(34)	141(11)	318(12)	300(13)	-3(10)	46(10)	-64(9)
C(35)	185(11)	289(12)	229(12)	27(9)	-4(9)	-115(9)
C(36)	274(12)	173(11)	293(13)	2(9)	65(10)	-40(9)
C(37)	190(11)	200(11)	252(12)	19(9)	82(9)	-16(8)
C(38)	146(10)	188(10)	110(9)	16(8)	20(8)	2(8)
C(39)	159(10)	280(12)	140(10)	-17(8)	24(8)	-36(9)
C(40)	263(12)	285(12)	159(11)	-29(9)	55(9)	-7(9)
C(41)	233(11)	291(12)	167(11)	34(9)	96(9)	54(9)

C(42)	169(10)	380(13)	183(11)	68(9)	59(8)	-11(9)
C(43)	183(10)	309(13)	131(10)	3(9)	27(8)	-73(9)
C(44)	147(10)	184(10)	144(10)	14(8)	2(8)	-12(8)
C(45)	178(11)	210(11)	216(11)	-10(9)	-47(9)	2(9)
C(46)	163(11)	263(11)	244(12)	-5(9)	-13(9)	35(8)
C(47)	252(12)	220(11)	239(12)	38(9)	49(9)	49(9)
C(48)	335(13)	195(11)	276(13)	46(9)	-12(10)	-77(10)
C(49)	172(11)	266(11)	209(11)	79(9)	-34(9)	-45(9)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for JSY01 (CCDC 186478).

	x	y	z	U_{iso}
H(1)	9816(10)	4305(14)	2285(9)	16(5)
H(3)	10389(10)	5719(14)	2035(9)	17(5)
H(4)	11413(9)	6588(13)	1754(8)	11(5)
H(5)	12429(10)	5593(14)	1574(9)	21(5)
H(6)	12407(11)	3733(14)	1653(9)	23(5)
H(7)	11402(9)	2866(13)	1923(8)	10(4)
H(9A)	10463(10)	671(13)	4476(8)	12(5)
H(9B)	9584(9)	654(13)	4410(8)	9(4)
H(11A)	10661(9)	3523(13)	4752(8)	11(4)
H(11B)	11130(10)	2485(13)	4691(9)	15(5)
H(12A)	9349(10)	3347(15)	4904(10)	27(5)
H(12B)	8929(11)	2237(14)	4767(9)	24(5)
H(12C)	9124(11)	2844(14)	4170(11)	28(6)
H(13A)	10847(11)	1444(14)	5632(9)	21(5)
H(13B)	9986(10)	1434(14)	5675(9)	20(5)
H(13C)	10424(11)	2475(16)	5798(10)	30(5)
H(16)	10071(10)	-1818(14)	2633(9)	15(5)
H(18)	8031(10)	-925(13)	2745(8)	8(5)
H(20A)	11098(10)	-681(15)	3675(10)	24(5)
H(20B)	11049(10)	415(15)	3364(9)	19(5)
H(20C)	11114(10)	-535(14)	2930(10)	22(5)
H(21A)	8321(16)	-2850(20)	2536(14)	74(9)
H(21B)	9019(15)	-3070(20)	2313(13)	65(10)
H(21C)	8379(15)	-2520(20)	1867(15)	75(9)
H(22A)	7763(11)	702(14)	3105(10)	25(5)
H(22B)	8310(11)	1646(16)	3143(10)	31(6)
H(22C)	8358(10)	947(13)	3792(10)	21(5)
H(25)	10944(10)	6406(14)	3699(9)	21(5)
H(27)	12584(10)	4396(14)	3476(9)	20(5)
H(29A)	9867(11)	4956(15)	4277(11)	32(6)
H(29B)	9524(11)	4626(16)	3545(10)	31(6)
H(29C)	9725(10)	5789(16)	3658(9)	25(5)
H(30A)	12207(14)	6900(20)	3197(14)	69(9)
H(30B)	12868(16)	6204(19)	3594(13)	71(9)
H(30C)	12390(14)	6880(20)	3930(14)	68(9)
H(31A)	12406(12)	2549(15)	3465(10)	32(6)
H(31B)	11608(10)	2164(13)	3054(10)	20(5)
H(31C)	11868(10)	2079(14)	3877(10)	22(5)
H(32)	7991(9)	1429(12)	439(9)	8(4)
H(33A)	7899(11)	1337(15)	1799(11)	27(6)
H(33B)	7484(10)	2196(15)	1336(10)	26(5)
H(34A)	6768(10)	875(14)	619(10)	24(5)
H(34B)	6678(11)	748(15)	1372(10)	31(6)
H(35A)	7475(11)	-701(15)	1561(11)	30(6)
H(35B)	6867(11)	-925(14)	918(9)	22(5)
H(36A)	7693(11)	-462(15)	207(11)	31(6)
H(36B)	8066(10)	-1285(15)	754(9)	19(5)
H(37A)	8802(10)	44(14)	1453(10)	23(5)

H(37B)	8914(11)	133(14)	686(10)	25(5)
H(38)	9690(9)	1368(13)	550(8)	6(4)
H(39A)	8836(10)	2577(14)	-539(9)	23(5)
H(39B)	8571(11)	1435(14)	-378(9)	23(5)
H(40A)	9617(10)	700(14)	-663(9)	17(5)
H(40B)	9191(10)	1345(14)	-1258(10)	19(5)
H(41A)	10053(10)	2690(14)	-989(10)	21(5)
H(41B)	10490(10)	1695(14)	-1053(9)	18(5)
H(42A)	10817(11)	1462(16)	172(10)	33(6)
H(42B)	11115(11)	2595(14)	-28(9)	24(5)
H(43A)	10470(10)	2801(13)	835(10)	17(5)
H(43B)	10012(9)	3407(14)	208(9)	13(5)
H(44)	8214(10)	3717(13)	1216(9)	16(5)
H(45A)	7448(11)	2941(15)	204(9)	25(5)
H(45B)	7931(11)	3569(15)	-263(11)	31(6)
H(46A)	6885(11)	4579(15)	-227(11)	32(6)
H(46B)	7052(11)	4554(15)	558(10)	30(6)
H(47A)	7399(10)	6218(14)	213(9)	18(5)
H(47B)	7868(10)	5685(13)	-225(10)	16(5)
H(48A)	8745(11)	6180(16)	754(10)	35(6)
H(48B)	8250(11)	5591(15)	1230(11)	32(6)
H(49A)	9321(11)	4594(15)	1130(10)	30(6)
H(49B)	9034(10)	4557(15)	331(10)	28(6)